

Quantum Antiferromagnetism of Fermions in Optical Lattices with Half-filled p -band

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We study Fermi gases in a three-dimensional cubic optical lattice with five fermions per site, i.e. the s -band is completely filled and the p -band with three-fold degeneracy is half filled. We show that, for repulsive interaction between fermions, the system will exhibit spin-3/2 antiferromagnetic order at low temperature. This conclusion is obtained both in strong interaction regime by strong coupling expansion, and in weak interaction regime by Hatree-Fock mean-field theory with analysis of the Fermi surface nesting. We also show that, in the strongly correlated regime, the Néel temperature for p -band antiferromagnetism is two to three orders of magnitudes higher than that of s -band, which is much more promising to be attained in cold atom experiments.

I. INTRODUCTION

Studying strong correlations in lattice Fermi gases has now become an emerging forefront of cold atom physics, mainly because of the flexibility of varying interactions and controlling filling number to access various quantum phases. One major effort pursued in many labs now is to use ultracold Fermi gases to simulate Hubbard model, which exhibits various metallic, insulating and superconducting phases, with different magnetic behaviors¹. Despite of huge efforts extending over several decades, there are still lots of controversial issues on this model, which hopefully cold atom experiments can shed light on.

The most solid conclusion of Hubbard model is drawn for a half-filled cubic lattice which says a spin-1/2 antiferromagnetic (AF) order exists for all range of repulsive interaction. For weak interaction, the AF order arises from the nesting geometry of Fermi surface, while for strong interaction, it is caused by the super-exchange interaction^{2,3,4,5}. Observing this AF order in cold atom experiments, especially in strong interaction regime, is considered as a hallmark of seeing strong correlations in lattice Fermi gases and the starting point for more ambitious goals along this direction.

On the other hand, in optical lattices physics can be much more richer than the single-band Hubbard model. When there are more than two fermions at one lattice site, fermions will start to occupy excited bands like the p -band. Unlike in condensed matter systems, there is no Jahn-Teller effect in optical lattices, so the three-fold orbital degeneracy of the p -band is well maintained.

Recently there are increasing theoretical and experimental interests in studying bosons in the p -band, where a host of intriguing quantum phenomena due to orbital degeneracy has been pointed out^{6,7,8,9,10}. We expect the physics of p -band fermions will be more easier for experimentally study, because the Pauli exclusion principle prevents the decay into the lower band. Thanks to the orbital degeneracy, p -band Fermi gases are expected to exhibit more diverse phases comparing to single-band Hubbard model. Nevertheless, the first step toward revealing these exciting phases is to understand the un-

frustrated spin order at half-filling. Here we consider a three-dimensional cubic lattice whose three degenerate p -bands are half filled by three fermions per site. (The s -band is already completely filled by another two fermions and do not need to be worried about.)

With the complexity in p -band model, even for half-filling there are issues not clear, for instance (i) whether the p -band fermi-surface still has some nesting properties which give rise to a magnetic instability in weak interaction regime; (ii) with multiple hopping channels in different orbitals and multiple choices of intermediate states, whether super-exchange processes can still yield a simple Heisenberg-type model as in the s -band situation; and (iii) as there are various types of orders due to orbital degrees of freedom, whether the strong and weak interaction regime share the same order or there is quantum phase transition in between. These questions will be answered in this work. The main results of this paper can be summarized as:

(I) In strong interaction regime, at each isolated site the ground state of three fermions in p -orbitals are spin-3/2 states with four-fold degeneracy due to the Hund's rule. The coupling between two neighboring spins is caused by virtual hopping of fermions, which gives rise to an isotropic spin-3/2 Heisenberg model:

$$\mathbf{H}_J = J_{\text{ex}} \sum_{\langle ij \rangle} \left(\vec{S}_i \vec{S}_j - \frac{1}{4} n_i n_j \right) \quad (1)$$

where \vec{S}_i is an on-site spin-3/2 operator. $J_{\text{ex}} > 0$ which means the ground state of this system has spin-3/2 antiferromagnetic order.

(II) In weak interaction regime, the Fermi surface of a half-filled p -band exhibits a perfect nesting symmetry, with the nesting momentum $\vec{\pi} = (\pi, \pi, \pi)$. Mean-field analysis shows this nesting will induce antiferromagnetic order at low-temperature, and the order parameter coincides with the $S = 3/2$ spin order in strong interaction regime. We also show that this order should be the only order parameter.

Based on (I) and (II), we anticipate that, despite the complexity with p -band orbital degeneracy, the half-filled

p -band Hubbard model exhibits only the spin-3/2 antiferromagnetic order for all range of interaction strength, and the system undergoes a *crossover* from weak to strong interaction, a situation similar to the half-filled single-band Hubbard model.

In the experiments of cold atoms in optical lattices, the major difficulty in achieving AF order in strongly correlated regime comes from the fact that the Néel temperature is very low because of the ultra-small energy scale of super-exchange interaction. In this work we show that in strong interaction regime the Néel temperature for p -band AF can reach a few nano-Kelvin, which is two to three orders of magnitude higher than that of s -band. Because of this we suggest to study p -band Fermi gas as a more realistic and promising route to reveal strongly correlated physics in optical lattices.

II. MODEL

The model for Fermi gases in optical lattices contains a nearest neighbor hopping \mathbf{H}_t and an on-site interaction \mathbf{H}_U . The hopping term \mathbf{H}_t can be written as:

$$\mathbf{H}_t = \sum_{i,s} \sum_{\alpha,\beta=x,y,z} T_{\beta}^{p_{\alpha}} c_{i,p_{\alpha},s}^{\dagger} c_{i+\hat{\beta},p_{\alpha},s} + \text{h.c.}, \quad (2)$$

Since optical lattice is a separable potential in three dimensions ($V_0(\sin^2 Kx + \sin^2 Ky + \sin^2 Kz)$), the hopping term conserves orbital index due to the orthogonality of wannier wave functions, and the hopping amplitude is anisotropic $T_{\beta}^{p_{\alpha}} = t\delta_{\alpha\beta} - t'(1 - \delta_{\alpha\beta})$ with $t, t' > 0$. And there is also no next nearest neighbor hopping⁴. Fig. 1(A) is a schematic of hoppings in the p -band. t is much larger than t' , for instance, for an optical lattice with the depth $V_0 = 11E_R$ ($E_R = \hbar^2 K^2/(2m)$ is the photon recoil energy), $t \approx 20t'$. For ultra-cold neutral gases, the

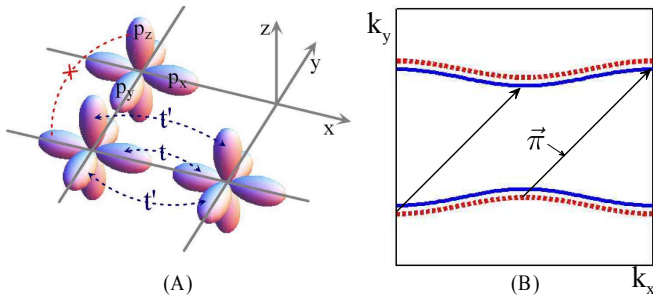


FIG. 1: (color on-line) (A) Schematic of fermion hopping in p -band. For a fermion in p_x orbital in i -site, its hopping amplitude to $i+\hat{x}$ site is t , to $i+\hat{y}$ -site and $i+\hat{z}$ site is t' ($t' \ll t$), and it can not hop to p_y (or p_z) orbital of its neighboring site. (B) Illustration of the p -band Fermi surface nesting at half-filling. Red line and blue line are Fermi surfaces in $k_x - k_y$ plane for $k_z = \pi/3$ and $k_z = -2\pi/3$, respectively. These two Fermi surfaces parallel with the nesting momentum $\vec{\pi} = (\pi, \pi, \pi)$ (the solid black arrow).

interaction is dominated by short-range s -wave repulsion $V(\mathbf{r}_{12}) = (4\pi\hbar^2 a_s/m)\delta(\mathbf{r}_1 - \mathbf{r}_2)$, which takes place between unlike spins only³. The on-site interaction \mathbf{H}_U then has the form

$$\mathbf{H}_U = \sum_i \left\{ U \sum_{\alpha} n_{i,p_{\alpha},\uparrow} n_{i,p_{\alpha},\downarrow} + W \sum_{\alpha \neq \beta} (n_{i,p_{\alpha},\uparrow} n_{i,p_{\beta},\downarrow} + c_{i,p_{\alpha},\uparrow}^{\dagger} c_{i,p_{\beta},\downarrow}^{\dagger} c_{i,p_{\alpha},\downarrow} c_{i,p_{\beta},\uparrow} + c_{i,p_{\alpha},\uparrow}^{\dagger} c_{i,p_{\alpha},\downarrow}^{\dagger} c_{i,p_{\beta},\downarrow} c_{i,p_{\beta},\uparrow}) \right\}, \quad (3)$$

$$U = \frac{4\pi\hbar^2 a_s}{m} \int d^3\mathbf{r} |w_{p_{\alpha}}(\mathbf{r})|^4 \quad (4)$$

$$W = \frac{4\pi\hbar^2 a_s}{m} \int d^3\mathbf{r} |w_{p_{\alpha}}(\mathbf{r})|^2 |w_{p_{\beta}}(\mathbf{r})|^2 \quad (5)$$

where $w_{p_{\alpha}}$ is the p_{α} -orbital wannier wave function. There are totally four terms due to s -wave interaction. The first term is the interaction within the same orbital, the second term is the interaction between unlike orbitals, the third term represents the spin exchange between unlike orbitals and the fourth term represents two fermions hopping processes from one orbital to another. Usually U is three times larger than W .

III. STRONG INTERACTION REGIME

When the on-site interaction is dominative, we shall first ignore the hopping term and calculate all the eigenstates of an isolated site. The results for three, four and two fermions per site are summarized in following Table I, II and III. As one can see from Table I, the low-energy Hilbert space is constituted by four spin-3/2 states. Because these spin states are symmetric superpositions of three atoms, their spatial wave functions have to be anti-symmetric and the interactions are completely quenched. In this limit, the system is a spin-3/2 Mott insulator¹¹.

$E = 0 (S = 3/2)$	$E = 3W (S = 1/2)$	$E \geq U$
$ \uparrow\uparrow\uparrow\rangle$	$(\uparrow\uparrow\downarrow\rangle - \uparrow\downarrow\uparrow\rangle)/\sqrt{2}$	double occupied states
$ \downarrow\downarrow\downarrow\rangle$	$(\downarrow\downarrow\uparrow\rangle - \downarrow\uparrow\downarrow\rangle)/\sqrt{2}$	
$(\downarrow\uparrow\uparrow\rangle + \uparrow\downarrow\uparrow\rangle + \uparrow\uparrow\downarrow\rangle)/\sqrt{3}$	$(\downarrow\downarrow\uparrow\rangle - \downarrow\uparrow\downarrow\rangle)/\sqrt{2}$	
$(\downarrow\uparrow\downarrow\rangle + \uparrow\downarrow\downarrow\rangle + \uparrow\downarrow\uparrow\rangle)/\sqrt{3}$	$(\uparrow\uparrow\downarrow\rangle - \uparrow\downarrow\uparrow\rangle)/\sqrt{2}$	

TABLE I: Eigenstates and eigenenergies of three fermions at an isolated site. In these three tables, we define that, for example, $|\downarrow\uparrow 0\rangle$ means p_x is double-occupied, p_y is occupied by a spin- \uparrow fermion, and p_z is empty.

The coupling of spins between neighboring sites can be obtained by taking the hopping term as the second-order perturbation with the Brillouin-Wigner approximation²:

$$\mathbf{H}_J = - \sum_e \mathcal{P}_G \mathbf{H}_t \mathcal{P}_e \frac{1}{\mathbf{H}_U} \mathcal{P}_e \mathbf{H}_t \mathcal{P}_G, \quad (6)$$

where \mathcal{P}_e means the projection into excited Hilbert space, and \mathcal{P}_G means the projection into $S = 3/2$ Hilbert space.

$E = U + 2W (S = 1)$	$E = U + 4W (S = 0)$
$ d \uparrow \uparrow\rangle, \uparrow \uparrow d\rangle, \uparrow \uparrow d\rangle, d \downarrow \downarrow\rangle,$ $ \downarrow \downarrow d\rangle, \downarrow \downarrow d\rangle, (d \uparrow \uparrow\rangle + d \downarrow \downarrow\rangle)/\sqrt{2}$ $(\uparrow \uparrow d\rangle + \downarrow \downarrow d\rangle)/\sqrt{2}$ $(\uparrow \uparrow d\rangle + \downarrow \downarrow d\rangle)/\sqrt{2}$	$(d \uparrow \downarrow\rangle - d \downarrow \uparrow\rangle)/\sqrt{2}$ $(\uparrow \uparrow d\rangle - \downarrow \downarrow d\rangle)/\sqrt{2}$ $(\uparrow \uparrow d\rangle - \downarrow \downarrow d\rangle)/\sqrt{2}$

TABLE II: Eigenstates and eigenenergies of four fermions at an isolated site.

$E = 0 (S = 1)$	$E = 2W (S = 0)$	$E \geq U - W$
$ 0 \uparrow \uparrow\rangle, \uparrow \uparrow 0\rangle, \uparrow \uparrow 0\rangle,$ $ 0 \downarrow \downarrow\rangle, \downarrow \downarrow 0\rangle, \downarrow \downarrow 0\rangle$ $(0 \uparrow \downarrow\rangle + 0 \downarrow \uparrow\rangle)/\sqrt{2}$ $(\uparrow \uparrow 0\rangle + \downarrow \downarrow 0\rangle)/\sqrt{2}$ $(\uparrow \downarrow 0\rangle + \downarrow \uparrow 0\rangle)/\sqrt{2}$	$(0 \uparrow \downarrow\rangle - 0 \downarrow \uparrow\rangle)/\sqrt{2}$ $(\uparrow \uparrow 0\rangle - \downarrow \downarrow 0\rangle)/\sqrt{2}$ $(\uparrow \uparrow 0\rangle - \downarrow \downarrow 0\rangle)/\sqrt{2}$ $(\uparrow \downarrow 0\rangle - \downarrow \uparrow 0\rangle)/\sqrt{2}$	double occupied states

TABLE III: Eigenstates and eigenenergies of two fermions at an isolated site.

To proceed we make following observations: (i) The virtual hopping processes only take place within the same orbital, otherwise the final state will have double occupancy, which should be projected out. For instance, if a p_x fermion hops from i -site to j -site, it must be followed by a p_x fermion hops from j -site to i -site. (ii) By using Table I, II and III one can show that only one type of excited states can be connected to the unperturbed ground states via hopping, which is the lowest energy states of four fermions ($S = 1$ and $E = U + 2W$) in one site and the lowest energy states of two fermions ($S = 1$ and $E = 0$) in its neighborhood¹². So the intermediate states always has energy $U + 2W$.

Because of (i-ii), \mathbf{H}_J on the link between i and $i + \hat{x}$ site reads

$$\sum_{p_\alpha} \frac{2|T_x^{p_\alpha}|^2}{U + 2W} \mathcal{P}_G \left(\sum_{ss'} c_{i,p_\alpha,s}^\dagger c_{i,p_\alpha,s'} c_{i+\hat{x},p_\alpha,s'}^\dagger c_{i+\hat{x},p_\alpha,s} \right) \mathcal{P}_G.$$

Note that

$$c_{i,p_\alpha,s}^\dagger c_{i,p_\alpha,s'} = \frac{1}{3} \left(\sum_{p_\beta} c_{i,p_\beta,s}^\dagger c_{i,p_\beta,s'} + \sum_{p_\beta} \Xi_{i,p_\alpha,p_\beta}^{s,s'} \right),$$

where

$$\Xi_{i,p_\alpha,p_\beta}^{s,s'} = c_{i,p_\alpha,s}^\dagger c_{i,p_\alpha,s'} - c_{i,p_\beta,s}^\dagger c_{i,p_\beta,s'}, \quad (7)$$

and with the help of Table I, one can show that

$$\mathcal{P}_G \Xi_{i,p_\alpha,p_\beta}^{s,s'} \mathcal{P}_G = 0 \quad (8)$$

$$\mathcal{P}_G \sum_{p_\beta} c_{i,p_\beta,s}^\dagger c_{i,p_\beta,s'} \mathcal{P}_G = \sum_{p_\beta} c_{i,p_\beta,s}^\dagger c_{i,p_\beta,s'}. \quad (9)$$

Then H_J on this link can be written as

$$\begin{aligned} & \sum_{p_\alpha} \frac{2|T_x^{p_\alpha}|^2}{9(U + 2W)} \sum_{ss'} \sum_{p_\beta} c_{i,p_\beta,s}^\dagger c_{i,p_\beta,s'} \sum_{p'_\beta} c_{i,p'_\beta,s}^\dagger c_{i,p'_\beta,s'} \\ &= \frac{1}{2} J_{\text{ex}} \sum_{p_\alpha, p_\beta} \sum_{s, s'} \left(c_{i,p_\alpha,s}^\dagger c_{i,p_\alpha,s'} \right) \left(c_{i+\hat{x},p_\beta,s'}^\dagger c_{i+\hat{x},p_\beta,s} \right) \end{aligned}$$

where

$$J_{\text{ex}} = 4(t^2 + 2t'^2)/(9U + 18W). \quad (10)$$

We now introduce \vec{S}_i as

$$\vec{S}_i = \frac{1}{2} \sum_{p_\alpha} \sum_{ss'} c_{i,p_\alpha,s}^\dagger \vec{\sigma}_{ss'} c_{i,p_\alpha,s'} \quad (11)$$

and $\vec{\sigma}$ are the Pauli matrices. Restricted in the low-energy Hilbert space, \vec{S}_i acts as $S = 3/2$ spin operator. Hence, we have shown the first main result that

In the strong interaction regime, the super-exchange processes induce an isotropic spin-3/2 Heisenberg model

$$\mathbf{H}_J = J_{\text{ex}} \sum_{\langle ij \rangle} \left(\vec{S}_i \vec{S}_j - \frac{1}{4} n_i n_j \right) \quad (12)$$

which describes the low-energy spin dynamics of p -band Mott insulator. $J_{\text{ex}} > 0$. Below Néel temperature, it will give rise to an antiferromagnetic long range order of $\langle S_i^+ \rangle = (-1)^i |\langle S_i^+ \rangle| \neq 0$

IV. WEAK INTERACTION REGIME

In this regime we use usual Hartree-Fock mean-field theory, for which the Hamiltonian is rewritten into momentum space. The hopping term can be written as:

$$\mathbf{H}_t = \sum_{\mathbf{k}, \alpha} \epsilon_{\mathbf{k}}^{p_\alpha} c_{p_\alpha, \mathbf{k}}^\dagger c_{p_\alpha, \mathbf{k}}, \quad (13)$$

where

$$\epsilon_{\mathbf{k}}^{p_\alpha} = 2t \cos k_\alpha - 2t' \sum_{\beta \neq \alpha} \cos k_\beta - \mu. \quad (14)$$

For half-filling, $\mu = 0$, and the Fermi surface for one of the p -bands is plotted in Fig. 1(B).

For performing mean-field decomposition, we reconstruct the interaction term \mathbf{H}_U as $\mathbf{H}_U^0 + \mathbf{H}_U'$, where

$$\mathbf{H}_U^0 = -V_1 \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \hat{\Delta}_{\mathbf{k}, \mathbf{q}}^\dagger \hat{\Delta}_{\mathbf{k}', \mathbf{q}}, \quad (15)$$

$$\mathbf{H}_U' = \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}}^{\alpha \neq \beta} \left(-V_2 \hat{\Gamma}_{\mathbf{k}, \mathbf{q}}^{\alpha \beta \dagger} \hat{\Gamma}_{\mathbf{k}', \mathbf{q}}^{\alpha \beta} - 2W \hat{\Sigma}_{\mathbf{k}, \mathbf{q}}^{\alpha \beta \dagger} \hat{\Sigma}_{\mathbf{k}', \mathbf{q}}^{\alpha \beta} \right) \quad (16)$$

with $V_1 = 3(U + 2W)$ and $V_2 = 2(U - W)/3$. Here we introduce

$$\hat{\Delta}_{\mathbf{k}, \mathbf{q}}^\dagger = \sum_{p_\alpha} S_{p_\alpha, p_\alpha, \mathbf{k}}^{\mathbf{q}+}/3, \quad (17)$$

and

$$\hat{\Gamma}_{\mathbf{k},\mathbf{q}}^{\alpha\beta\dagger} = (S_{p_\alpha,p_\alpha,\mathbf{k}}^{\mathbf{q}+} - S_{p_\beta,p_\beta,\mathbf{k}}^{\mathbf{q}+})/2, \quad (18)$$

$$\hat{\Sigma}_{\mathbf{k},\mathbf{q}}^{\alpha\beta\dagger} = (S_{p_\alpha,p_\beta,\mathbf{k}}^{\mathbf{q}+} + S_{p_\beta,p_\alpha,\mathbf{k}}^{\mathbf{q}+})/2, \quad (19)$$

where $S_{p_\alpha,p_\beta,\mathbf{k}}^{\mathbf{q}+} = c_{\mathbf{k},p_\alpha,\uparrow}^\dagger c_{\mathbf{k}+\mathbf{q},p_\beta,\downarrow}$ is the spin lifting operator. As illustrated in Fig. 1(B), each of three p -band Fermi-surfaces exhibits nesting symmetry with the nesting momentum $\vec{\pi} = (\pi, \pi, \pi)$ at half-filling. It means that for each \mathbf{k} at Fermi surface, $\mathbf{k} + \pi$ also locates at Fermi surface, therefore, the maximum contribution to \mathbf{H}_U comes from $\mathbf{q} = \vec{\pi}$. For this reason we only consider $\mathbf{q} = \vec{\pi}$ component in the mean-field approximation, and we introduce three order parameters which are $\Delta = V_1 \sum_{\mathbf{k}} \langle \hat{\Delta}_{\mathbf{k},\pi} \rangle$, $\Gamma = V_2 \sum_{\mathbf{k}} \langle \hat{\Gamma}_{\mathbf{k},\pi}^{\alpha\beta} \rangle / 3$ and $\Sigma = 2W \sum_{\mathbf{k}} \langle \hat{\Sigma}_{\mathbf{k},\pi}^{\alpha\beta} \rangle$, where Γ and Σ are independent of index α, β because of the permutation symmetry between orbitals. Note that Δ is the same spin order as in strong interaction regime, we separate the mean-field Hamiltonian into two parts as $\mathbf{H}_{\text{MF}} = \mathbf{H}_0 + \mathbf{H}'$ where

$$\mathbf{H}_0 = \sum_{\mathbf{k}} \left[\sum_{p_\alpha,\sigma} \epsilon_{\mathbf{k}}^{p_\alpha} c_{\mathbf{k},p_\alpha,\sigma}^\dagger c_{\mathbf{k},p_\alpha,\sigma} + (\Delta \hat{\Delta}_{\mathbf{k}}^\dagger + \text{h.c.}) \right] + \frac{\Delta^2}{V_1}$$

and

$$\mathbf{H}' = \sum_{\mathbf{k}} \left[\sum_{\alpha \neq \beta} \hat{\Sigma}_{\mathbf{k}}^{\alpha\beta\dagger} + \text{h.c.} \right] + \frac{\Gamma^2}{V_2} + \frac{\Sigma^2}{2W}$$

Note that \mathbf{H}' does not contain $\hat{\Gamma}$ -terms because they all cancel out due to the permutation symmetry of three orbitals, therefore $\Gamma = 0$.

Because the three orbitals are now separable in \mathbf{H}_0 , it can be easily diagonalized by Bogoliubov transformation

$$\mathbf{H}_0 = \sum_{\mathbf{k},\alpha} \xi_{\mathbf{k}}^{p_\alpha} (\gamma_{\mathbf{k},p_\alpha}^\dagger \gamma_{\mathbf{k},p_\alpha} + \eta_{\mathbf{k},p_\alpha}^\dagger \eta_{\mathbf{k},p_\alpha} - 1) + \frac{\Delta^2}{V_1}, \quad (20)$$

where

$$\xi_{\mathbf{k}}^{p_\alpha} = \sqrt{(\epsilon_{\mathbf{k}}^{p_\alpha} - \epsilon_{\mathbf{k}+\vec{\pi}}^{p_\alpha})^2 / 4 + (\Delta/3)^2}, \quad (21)$$

and $\gamma_{\mathbf{k},p_\alpha}$ and $\eta_{\mathbf{k},p_\alpha}$ are quasi-particle operators¹³. The equation for Δ is

$$\frac{1}{V_1} = \sum_{\mathbf{k},p_\alpha} \frac{\tanh(\xi_{\mathbf{k}}^{p_\alpha} \beta / 2)}{\xi_{\mathbf{k}}^{p_\alpha}}, \quad (22)$$

the solution of which yields non-zero value of Δ and the critical temperature for having non-zero Δ .

Next we shall examine whether there will be symmetry breaking of Σ also, for which we treat \mathbf{H}' as perturbation on top of \mathbf{H}_0 , and the energy can be expanded in powers of Σ as $E_{\text{MF}} = E_0(\Delta) + \chi(\Delta)\Sigma^2 + O(\Sigma^4)$. So whether there is an instability for developing finite Σ depends on the sign of χ . Straightforward calculation shows that

$$\chi(\Delta) = - \sum_{\mathbf{k},\alpha \neq \beta} \frac{|\tau_{\mathbf{k}}^{\alpha\beta}|^2}{2(\epsilon_{\mathbf{k}}^{p_\alpha} + \xi_{\mathbf{k}+\vec{\pi}}^{p_\beta})} + \sum_{\mathbf{k},\alpha} \frac{V_1}{2W} \frac{1}{\xi_{\mathbf{k}}^{p_\alpha}}, \quad (23)$$

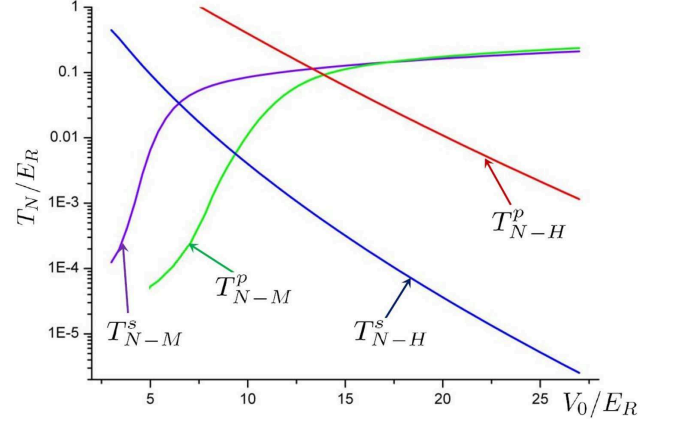


FIG. 2: (color on-line) Néel temperature T_N as a function of optical lattice depth V_0 . Four curves are p -band T_N from Heisenberg model T_{N-H}^p , from mean-field theory T_{N-M}^p ; s -band T_N from Heisenberg model T_{N-H}^s , from mean-field theory T_{N-M}^s , respectively. For parameters, we use ^{40}K in optical lattices as an example¹⁴. The lattice spacing $\lambda = 1064\text{nm}$, $K = \pi/\lambda$ and $a_s = 15\text{nm}$. The energy units is taken as E_R , which corresponds to $0.21\mu\text{K}$.

where $\tau_{\mathbf{k}}^{\alpha\beta} = v_{\mathbf{k},p_\alpha} v_{\mathbf{k}+\vec{\pi},p_\beta} - u_{\mathbf{k},p_\alpha} u_{\mathbf{k}+\vec{\pi},p_\beta}$ ¹³. We numerically compute Eq. (23) and find that it is always positive, which indicates that there will be no symmetry breaking of Σ . Mathematically, it is because $\xi_{\mathbf{k},p_\alpha} \neq \xi_{\mathbf{k}+\vec{\pi},p_\beta}$ except for a few specific points in momentum space. In the limit of $\Delta \rightarrow 0$, the first term in the r.h.s. of Eq. (23) diverges only around those a few points, while the second term diverges around the whole Fermi surface, hence the second term will always be dominative and the whole summation is positive. Physically, it is because the AF instability crucially relies on the nesting of Fermi surface, and the fact that there is no nesting between two different p -bands prevents inter-orbital spin order. Hence we have reached the second main result that

In the weak interaction regime, the only spin order at low-temperature is $\Delta = \langle \sum_{\mathbf{k},\alpha} c_{\mathbf{k},p_\alpha,\uparrow}^\dagger c_{\mathbf{k}+\vec{\pi},p_\alpha,\downarrow} \rangle \neq 0$ and this order coincides with that in strong interaction regime.

V. NÉEL TEMPERATURE

Here we first calculate the wannier functions in an optical lattice potential and use them to deduce the parameters t, t', U and W in our model. Then, we calculate the Néel temperature given by Heisenberg model of Eq.(12) T_{N-H} , which is $1.276 J_{\text{ex}} S(S+1)$,⁴ and also calculate T_{N-M} given by mean-field theory by solving equation (22) for the onset of non-zero Δ . We display our calculation of these two T_N for both half-filled p -band and s -band in Fig. 2. T_{N-H} decreases as the increase of the lattice height while T_{N-M} increases as the increase of the lattice height.

For small V_0 , $T_{N-M} \ll T_{N-H}$, the AF order is caused by

mean-field effect, while for large V_0 where $T_{N-H} \ll T_{N-M}$, the AF order is driven by super-exchange processes and the system is in strongly correlated regime. The regime where T_{N-M} and T_{N-H} cross is the crossover regime from weak to strong interactions, where both two methods will fail, and more advanced numerical technique like DMFT and QMC is required in order to give accurate Néel temperature⁵. We will leave this for further investigation. However, the key point is that the s-band T_{N-H} is already of the order of 0.1nK when the lattice height enters the strongly correlated regime of great experimental interests, and it decreases to below 10^{-2} nK rapidly as V_0 increases, while the p-band T_{N-H} remains the order of 1nK even when V_0 increases to $\sim 20E_R$. It is simply because the wannier wave function in p-band is much more extended, its hopping amplitude t is one to two orders larger than that of s-band, which consequently leads to much larger J_{ex} .

In addition to higher Néel temperature, the spin-3/2 of p-band AF state could have a better signal-to-noise ratio than s-band spin-1/2 AF. All these provide great advantage for experimental study of quantum AF and its related phenomena due to super-exchange. Besides, we leave the effect of trapping potential to future investigation which may introduce shell structure in density profile and the finite size effect into the problem.

We hope that this work will open up a new route for studying strongly correlated Fermi gases in optical lattices, and be bases for future efforts along this direction.

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¹² It is because the lowest energy states in each table are all constructive superposition of different states, while other states are destructive superposition.

¹³ $\gamma_{\mathbf{k},p_\alpha} = u_{\mathbf{k},p_\alpha} c_{\mathbf{k},p_\alpha,\uparrow} - v_{\mathbf{k},p_\alpha} c_{\mathbf{k}+\mathbf{q},p_\alpha,\downarrow}$ and $\eta_{\mathbf{k},p_\alpha}^\dagger = v_{\mathbf{k},p_\alpha} c_{\mathbf{k},p_\alpha,\uparrow} + u_{\mathbf{k},p_\alpha} c_{\mathbf{k}+\mathbf{q},p_\alpha,\downarrow}$, where $u_{\mathbf{k},p_\alpha}/v_{\mathbf{k},p_\alpha} = (1 \pm \epsilon_{\mathbf{k},p_\alpha}/\xi_{\mathbf{k},p_\alpha})/2$.

¹⁴ M Köhl, H. Moritz, T. Stöferle, K. Günter, and T. Esslinger, Phys. Rev. Lett. **94**, 080403 (2005)